

Effects of phonon interaction on the pairing in the high- T_c superconductors

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We study the effects of phonon interaction on the superconducting pairing in the background of a d-wave gap, mediated by antiferromagnetic (AFM) spin fluctuations, using coupled BCS gap equations. We found that phonon interaction can induce a s-wave component to the d-wave gap in the (D+S) form with an interaction anisotropy and in the (D+iS) form without anisotropy, respectively. In either case, however, T_c is not enhanced compared to the pure d-wave pairing without phonon interaction. On the other hand, anisotropic phonon interaction can dramatically enhance the d-wave pairing itself and therefore T_c , together with the AFM spin fluctuation interaction. This ($D_{AFM} + D_{ph}$) type pairing exhibits strongly reduced isotope coefficient despite the large enhancement of T_c by phonon interaction. Finally, we study the combined type of ($D_{AFM} + D_{ph} + iS$) gap and calculate the penetration depth and specific heat to be compared with the experiments.

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I. INTRODUCTION

The problems of the high T_c superconductors (HTSC) have been mostly focused on the electronic correlations and phonons were usually considered as a secondary player at best. However, recent Angle Resolved Photoemission Spectroscopy (ARPES) experiments revived the interest of the possibly important role of phonons in the high- T_c cuprates (HTC)¹. In particular, the systematic measurements and analysis² of the kink structures in the quasiparticle dispersion near the Fermi surface (FS) proved that: (1) the origin of the kink is electron-phonon coupling and its coupling is very strong, (2) the typical energy of the phonon(s) is $\sim 40 - 70$ meV, and (3) the coupling matrix is quite anisotropic. Therefore, it is currently a pressing question what possible roles and effects, in particular, for the superconducting (SC) pairing, the phonon(s) can do in the HTC.

Although the SC gap symmetry in the high- T_c cuprates is well established as a d-wave by most experiments, there are also continuous experimental reports such as tunnelling conductance³, penetration depth measurements⁴, etc that provide rather convincing evidences for a small magnitude of a s-wave component in addition to the dominant d-wave SC gap in some of HTC compounds. And it is well known that phonons mediate an attractive interaction between electrons and lead to an isotropic s-wave gap. Therefore, more sharpened question will be: is it possible to reconcile a d-wave gap and a s-wave gap together? and in that case, what is the role of phonon(s)?

While there is no consensus yet on the pairing mechanism for the d-wave gap in HTC, in this paper we assume that the AFM spin fluctuations is the mediating glue for d-wave gap⁵. The key ingredient of this mechanism is that the sign changing character of the d-wave gap turns the all positive definite potential of the AFM spin fluctuations mediated interaction (we will call it "AFM interaction" for short from now), in momentum space and in spin singlet channel, into an effectively attractive pairing interaction. From this point of view, it is clear that the phonon interaction and AFM interaction are antagonistic and difficult to work together for making a pairing

because they tend to promote a different symmetry of the SC gap each other.

An easy way to reconcile the d-wave and s-wave gap with two different pairing interactions would be to invoke two separate bands for each gap⁶. The similar idea for the two s-wave gaps was very successful for MgB_2 ⁷ because there two well separated bands exist. However, in HTSC, numerous experiments, in particular ARPES measurements⁸, show that there is only one main band crossing FS. Then any idea of having s-wave and d-wave gaps in the single band, induced by two very different pairing interactions, seems too naive. However, if the coupling matrix of phonon interaction possesses a strong anisotropy, this combined pairing problem is not a trivial one and needs systematic investigation with a traceable formulation. This problem has been already studied by many authors with different techniques and aims^{9,10,11}. In this paper, we took a simplest approach and studied the coupled gap equations for multiple gaps of a single band with two pairing interactions, i.e., AFM interaction and anisotropic phonon interaction, within the BCS framework. More justification for this approach will be discussed in the next section. By numerical solutions, we extensively investigated the necessary conditions of the strength and the degree of anisotropy of phonon interaction for various multigap solutions.

We found that the (D+S) and (D+iS) type solutions are indeed possible with a proper degree of anisotropy of phonon interaction for each case. However, T_c is not enhanced at all in these cases even though an additional s-wave component is formed due to the phonon interaction. Other interesting possibility is that the anisotropic phonon interaction can induce an additional d-wave component (D_{ph}) to the AFM interaction induced d-wave component (D_{AFM}). As a result, T_c is dramatically enhanced due to the phonon interaction. We then derived an analytic T_c equation for this ($D_{AFM} + D_{ph}$) case and showed that phonon isotope effect can be strongly reduced due to the interplay between the AFM and phonon interactions despite the large increase of T_c by phonon. This result can explain a long standing puzzle of the small phonon isotope effect in HTSC. In view of experiments², the best anisotropic phonon can be the B_{1g} buckling phonon mode which fulfills

all necessary qualifications for our model. Similar conclusion was obtained by other authors¹⁰ using different approaches. We emphasize that the final effect of phonons in HTC compounds should be judged by an average effect of all important phonons together, which is beyond the scope of this paper.

Finally, we also considered the combined type of $(D_{AFM} + D_{ph} + iS)$ gap which is a very natural solution of the coupled gap equations and shows features such as (1) large enhanced T_c , and (2) appearance of a s-wave component at low temperatures. This type of gap will be a possible solution for the tunnelling conductance experiment in YBCO³. Calculations of superfluidity density also demonstrated that $(D_{AFM} + D_{ph} + iS)$ gap can explain the non-monotonic temperature dependence of the penetration depth measurements in YBCO and LSCO compounds⁴.

II. FORMALISM

The interplay between phonons and electronic correlations in HTSC has been studied by numerous authors using different theoretical approaches and models^{9,10,11}. In this paper, we took a simple minded approach with a specific question for this problem. Experiments tell us that, after all correlation effects taken place, the quasiparticles (q.p.) remain to form a fermi surface (FS)⁸. And quite detailed properties of the AFM spin fluctuations and symmetry allowed phonons are experimentally measured¹; these measured bosonic fluctuations are final outcomes after all interplays between them and correlation effects. Now on the phenomenological basis, we consider a q.p. band and the AFM spin fluctuations as a dominant pairing interaction. In addition to that we add anisotropic phonon interactions and we study the pairing instability of the model for several possible types of multi-gap solution using a generalized BCS gap equations. In this approach, still remaining interplay between spin fluctuations and phonons is ignored. The results of this paper should be taken with this caveat. The Hamiltonian is written as

$$H = \sum_{k\sigma} \epsilon(k) c_{k\sigma}^\dagger c_{k\sigma} + \sum_{kk' \uparrow \downarrow} V_{AFM}(k, k') c_{k\uparrow}^\dagger c_{-k\downarrow}^\dagger c_{k'\downarrow} c_{-k'\uparrow} + \sum_{kk' \uparrow \downarrow} V_{ph}(k, k') c_{k\uparrow}^\dagger c_{-k\downarrow}^\dagger c_{k'\downarrow} c_{-k'\uparrow} \quad (1)$$

where $\epsilon(k)$ is the dispersion of the quasiparticles created by $c_{k\sigma}^\dagger$ as standard notation. $V_{AFM}(k, k')$ and $V_{ph}(k, k')$ are the effective interactions, for the singlet superconducting pairing channel, originating from the AFM spin fluctuations and phonon(s), respectively. For traceable numerical calculations, we further simplify the above Hamiltonian as follows. The real two dimensional FS is simplified as a circular FS and the interactions are also modelled accordingly as follows.

$$V_{AFM}(\Delta\phi) = V_M \frac{\phi_0^2}{(\Delta\phi \pm \phi_{AFM})^2 + \phi_0^2} \quad (2)$$

and

$$V_{ph}(\Delta\phi) = \begin{cases} -V_P & \text{for } |\Delta\phi| < \phi_{AN} \\ 0 & \text{for } |\Delta\phi| > \phi_{AN} \end{cases} \quad (3)$$

where $\Delta\phi = \phi - \phi'$ and $\phi_{AFM} = \pi/2$ representing the exchanged momentum $\mathbf{k} - \mathbf{k}'$ and the AFM ordering vector \mathbf{Q} in the circular FS, respectively. V_M and V_P are chosen to be positive, so that V_{AFM} is all repulsive and V_{ph} is all attractive in momentum space.

The property of the AFM interaction with a short range correlation is simulated with the inverse correlation length parameter ϕ_0 ($\lambda = (\pi a/\sqrt{2})\phi_0$). In this paper, we chose $\phi_0=1$ ($\lambda \sim 2a$) for all numerical calculations, which is quite a short range AFM correlation. The degree of anisotropy of the phonon interaction is controlled by the anisotropy angle parameter ϕ_{AN} which restricts the scattering angle between incoming and outgoing q.p momenta; for example, $\phi_{AN} = \pi$ would allow a perfectly isotropic interaction. The phonon interaction $V_{ph}(\phi - \phi')$, however, does not restrict the incoming (ϕ) and outgoing momenta (ϕ'). Now the reduced BCS Hamiltonian in the mean field theory can be written as

$$H = \sum_{\phi\xi\sigma} \epsilon(\xi) c_{\phi\xi\sigma}^\dagger c_{\phi\xi\sigma} + \sum_{\phi\xi} \Delta_{AFM}^*(\phi) c_{\phi\xi\downarrow} c_{-\phi\xi\uparrow} + \sum_{\phi\xi} \Delta_{ph}^*(\phi) c_{\phi\xi\downarrow} c_{-\phi\xi\uparrow} \quad (4)$$

where $\Delta_{AFM}(\phi)$ is the SC gap function induced by V_{AFM} and $\Delta_{ph}(\phi)$ is the one induced by V_{ph} . The two gap functions $\Delta_{AFM}(\phi)$ and $\Delta_{ph}(\phi)$ may or may not have the same symmetry. After diagonalizing the above Hamiltonian we obtain two self-consistent equations as

$$\Delta_{AFM}(\phi) = \sum_{\phi'\xi} V_{AFM}(\phi - \phi') < c_{\phi\xi\downarrow} c_{-\phi\xi\uparrow} >, \quad (5)$$

$$\Delta_{ph}(\phi) = \sum_{\phi'\xi} V_{ph}(\phi - \phi') < c_{\phi\xi\downarrow} c_{-\phi\xi\uparrow} >. \quad (6)$$

Similar coupled gap equations were studied in previous studies⁶. The key difference is that our model has only one band. Then because the same band electrons should form the multigaps, there is severe competition between different gaps and more constraint to allow multigap solutions. In the next sections, we will consider several possible multigap solutions of the above coupled gap equations.

A. (D+S) case

In this case, we assume $\Delta_{AFM}(\phi) = \Delta_d \cos(2\phi)$ and $\Delta_{ph}(\phi) = \Delta_s$. This leads to the two coupled gap equations as follows.

$$\Delta_d(\phi) = - \sum_{\phi'} V_{AFM}(\phi - \phi') \Delta_t(\phi') \chi(\phi', \omega_{AFM}(\mathbf{r}))$$

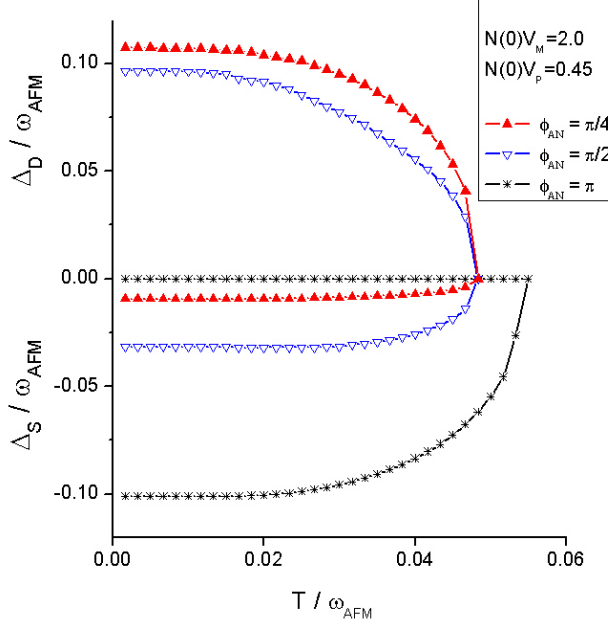


FIG. 1: (Color online) (D+S) case. Calculated magnitudes of d-wave components (Δ_D/ω_{AFM}) and s-wave components (Δ_S/ω_{AFM}) for different anisotropy angles $\phi_{AN} = \pi/4, \pi/2$, and π . For all cases $N(0)V_M = 2.0$, $N(0)V_P = 0.45$ and $\omega_{ph}/\omega_{AFM} = 0.5$.

$$\Delta_s(\phi) = - \sum_{\phi'} V_{ph}(\phi - \phi') \Delta_t(\phi') \chi(\phi', \omega_p), \quad (8)$$

$$\chi(\phi', \omega_{AFM,ph}) = N(0) \int_0^{\omega_{AFM,ph}} d\xi \frac{\tanh(\frac{E(\phi')}{2T})}{E(\phi')} \quad (9)$$

where $E(\phi) = \sqrt{\xi^2 + \Delta_t^2(\phi)}$, and $\Delta_t(\phi) = (\Delta_d \cos(2\phi) + \Delta_s)$ is the total gap function. $N(0)$ is the density of states (DOS) at FS and $\omega_{AFM,ph}$ are the BCS energy cutoffs of each pairing interactions V_{AFM} and V_{ph} , respectively. Nonzero value of Δ_s reduces the symmetry S_4 of the pure d-wave gap to C_2 ; namely, the nodal points shift away from diagonal directions and the sizes of the positive lobe and negative lobe of the total gap function $\Delta_t(\phi)$ become different. We found that the coexistence of d- and s-wave gaps is possible only when $V_{ph}(\phi - \phi')$ is strongly anisotropic; the minimum anisotropy of the phonon interaction is $\phi_{AN} \leq \pi/2$ for our model interaction of Eq.(3).

Fig.1 shows typical results of the (D+S) gap solution. The normalized d-wave gap Δ_D/ω_{AFM} and the s-wave gap Δ_S/ω_{AFM} are plotted for different values of anisotropy angle $\phi_{AN} = \pi/4, \pi/2$ and π with fixed values of coupling constants $N(0)V_M = 2$ and $N(0)V_P = 0.45$. The effective dimensionless coupling constants $\lambda_{AFM,ph}$ are smaller than these values which is defined below as a projected average with a SC gap function.

$$\lambda_{AFM,ph} = N(0) \frac{\sum_{\phi, \phi'} V_{AFM,ph}(\phi - \phi') \eta(\phi) \eta(\phi')}{\sum_{\phi} \eta^2(\phi)} \quad (10)$$

where $\eta(\phi) = \cos(2\phi)$ for d-wave gap and $\eta(\phi) = 1$ for s-wave gap. For the chosen potential strengths $N(0)V_M = 2$ and $N(0)V_P = 0.45$ in Fig.1, the effective coupling strengths are $\lambda_{AFM,D} = 0.332$ and $\lambda_{ph,S} = 0.450, 0.338, 0.198$ for $\phi_{AN} = \pi, \pi/2, \pi/4$, respectively.

When $\phi_{AN} = \pi$ (corresponding to a perfectly isotropic phonon interaction), solution is either a pure d-wave or a pure s-wave gap primarily depending on the strength of λ_{AFM} and λ_{ph} ; the final dominant instability is determined not only by the interaction strengths but also with the cutoff energy scales ω_{AFM} and ω_{ph} . In this case, $\lambda_{ph,S} (=0.450)$ is much bigger than $\lambda_{AFM,D} (=0.332)$, therefore a pure s-wave gap becomes a solution. Only when $\phi_{AN} \leq \pi/2$ and $\lambda_{ph,S}$ is not dominant over $\lambda_{AFM,D}$, a s-wave gap component can coexist with a d-wave component. When these conditions satisfied, no matter how weak the phonon interaction is, a finite s-wave component coexists over the entire temperatures and shares the same transition temperature T_c . Also this T_c remains the same as the pure d-wave T_{c0} without the phonon interaction, regardless of the presence of Δ_S and its magnitude. This somewhat unexpected result can be understood from the coupled gap equations Eq.(7-8). As far as the d-wave component is nonzero, that is the dominant pairing gap and T_c is determined solely by the d-wave gap equation Eq.(7) in the limit of $\Delta_D, \Delta_S \rightarrow 0$. In the opposite limit, namely, when $\lambda_{ph,S}$ is dominant over $\lambda_{AFM,D}$, then even if $\phi_{AN} \leq \pi/2$, the d-wave gap is entirely suppressed and T_c is determined solely by the s-wave gap equation Eq.(8).

In Fig.2 we fixed the anisotropy angle $\phi_{AN} (= \pi/4)$ and (9) changed the coupling strength of phonon $N(0)V_P (=0.7, 0.9, 1.1)$. The variation of the magnitude of the s-wave gap Δ_S can be understood with the effective coupling strength of $\lambda_{ph,S} (=0.31, 0.39, 0.48)$, respectively compared to $\lambda_{AFM,D} (=0.332)$ as in Fig.1. One peculiar feature occurs when $N(0)V_P = 0.9$ ($\lambda_{ph,S}=0.39$)(down triangles). The higher transition temperature $T_{c,high}$ is understood as the coexistence cases of Fig.1; although $\lambda_{ph,S} (=0.39) > \lambda_{AFM,D} (=0.332)$, the fact $\omega_{AFM} > \omega_{ph}$ makes the d-wave pairing still slightly dominant at high temperatures. But at lower temperature one more transition occurs where the d-wave gap collapses to zero and the s-wave gap component makes a sudden increase. This abrupt change of gaps is a first order transition and indicates that there are two competing local minima in the free energy. With temperature the global minimum changes from one local minimum to the other local minimum. This peculiar behavior is due to the closeness between $\lambda_{AFM,D}$ and $\lambda_{ph,S}$, and yet the distance of the energy scale between $\omega_{AFM} = 1$ and $\omega_P = 0.5$ as we have chosen in our calculations (all energy scales are normalized by ω_{AFM} in this paper) in this particular case. This is a rather artificial result of our model; nevertheless, it is an interesting behavior of the (D+S) type gap equations of Eq.(7-8).

The summary for the (D+S) type gap is: (1) The mixed type gap solution is possible if the phonon interaction has a

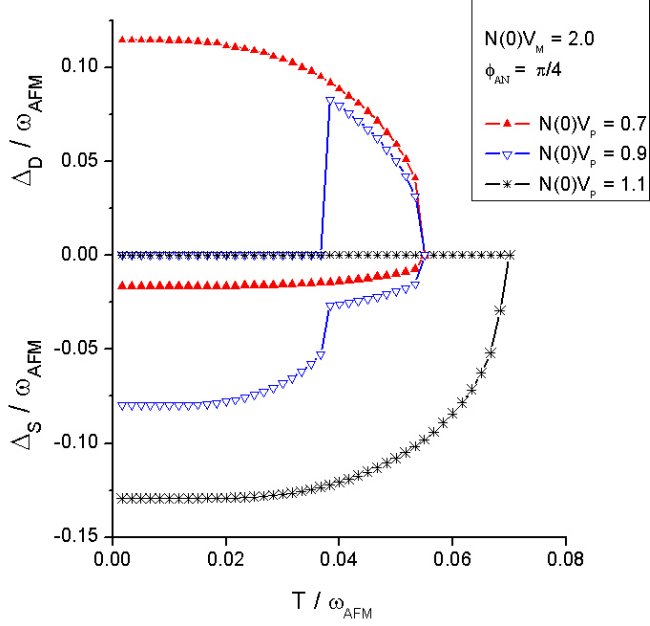


FIG. 2: (Color online) (D+S) case. Calculated magnitudes of d-wave components (Δ_D/ω_{AFM}) and s-wave components (Δ_S/ω_{AFM}) for different strength of phonon interaction $N(0)V_P = 0.7, 0.9$, and 1.1 . For all cases $N(0)V_M = 2.0$, $\phi_{AN} = \pi/4$ and $\omega_{ph}/\omega_{AFM}=0.5$.

proper anisotropy and its coupling strength is subdominant to the d-wave pairing strength; (2) T_c is not enhanced as far as the d-wave gap remains finite regardless of the presence and magnitude of the s-wave gap component.

B. (D+iS) case

In this case, we assume $\Delta_{AFM}(k) = \Delta_d \cos(2\phi)$ and $\Delta_{ph} = i\Delta_s$. Accordingly, $\Delta_t(\phi) = \Delta_d \cos(2\phi) + i\Delta_s$ and $E(\phi) = \sqrt{\xi^2 + \Delta_d^2(\phi) + \Delta_s^2}$. The gap equations are

$$\Delta_d(\phi) = - \sum_{\phi'} V_{AFM}(\phi - \phi') \Delta_t(\phi') \chi(\phi', \omega_{AFM}) \quad (11)$$

$$i\Delta_s(\phi) = - \sum_{\phi'} V_{ph}(\phi - \phi') \Delta_t(\phi') \chi(\phi', \omega_{ph}) \quad (12)$$

The main difference from the (D+S) case is that because of the phase i between $\Delta_d(\phi)$ and Δ_s , two gaps are only indirectly coupled through the quasiparticle energy $E(\phi)$ in the pair susceptibility $\chi(\phi, \omega_{M,ph})$. Therefore the coupling of two gaps is much smoother than the (D+S) case. One consequence of it is that the gap equations can allow two transition temperatures $T_{c,D}$ and $T_{c,S}$ for each gap Δ_D and Δ_S , respectively. This feature is shown in Fig.3 where $N(0)V_M = 2.0$ ($\lambda_{AFM,D} = 0.332$) and $N(0)V_P = 0.55$ are fixed and the anisotropy angle of phonon interaction ϕ_{AN} is varied as $\pi/4$, $\pi/2$, and π (correspondingly $\lambda_{ph,S} = 0.243, 0.414$ and 0.55).

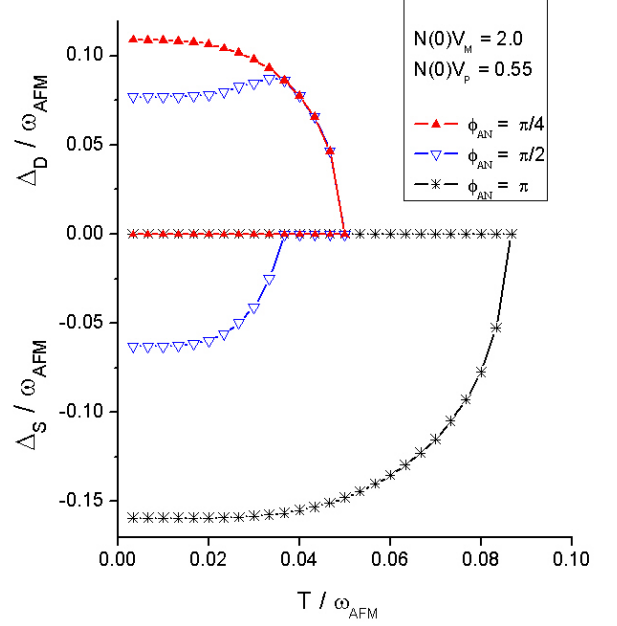


FIG. 3: (Color online) (D+iS) case. Calculated magnitudes of d-wave components (Δ_D/ω_{AFM}) and s-wave components (Δ_S/ω_{AFM}) for different anisotropy angles $\phi_{AN} = \pi/4, \pi/2$, and π . For all cases $N(0)V_M = 2.0$, $N(0)V_P = 0.55$ and $\omega_{ph}/\omega_{AFM}=0.5$.

Main features are summarized as: (1) when $\lambda_{ph,S}$ is too weak, the effect of phonon interaction is totally ignored and the gap and T_c is solely determined by the AFM interaction (see $\phi_{AN} = \pi/4$ case). (2) when $\lambda_{ph,S}$ is much stronger than $\lambda_{AFM,D}$, the d-wave gap is totally suppressed and the gap and T_c is determined solely by phonon interaction (see $\phi_{AN} = \pi$ case). This behavior is similar to the (D+S) case. (3) when the effective coupling strengths are comparable, namely $\lambda_{AFM,D} \approx \lambda_{ph,S}$, both d-wave and s-wave gaps have separate transition temperatures $T_{c,D}$ and $T_{c,S}$ and two gaps can coexist at low temperatures (see $\phi_{AN} = \pi/2$ case). In this case, $T_{c,D}$ is always higher transition temperature and this transition temperature is just the same as the pure d-wave T_{c0} without phonon interaction. At the lower transition temperature $T_{c,S}$, the s-wave gap $i\Delta_S$ appears and the magnitude of d-wave gap Δ_D accordingly decreases.

To clarify the roles of the anisotropy and the strength of phonon interaction, in Fig.4 we fixed anisotropy angle as $\phi_{AN} = \pi$, which simulates a perfectly isotropic phonon interaction, and varied the interaction strength. Fig.4 shows the results of these calculations. With $N(0)V_M = 2.0$ ($\lambda_{AFM,D} = 0.332$), we varied $N(0)V_P$ ($= 0.3, 0.4, 0.5$; accordingly $\lambda_S = 0.3, 0.4, 0.5$). This plot demonstrates that the anisotropy of phonon interaction doesn't play a particular role in the case of the (D+iS) type gap. The mixed gap solution of the (D+iS) type is still possible when $\lambda_{AFM,D}$ and $\lambda_{ph,S}$ are of the comparable strength regardless of the anisotropy of phonon interaction.

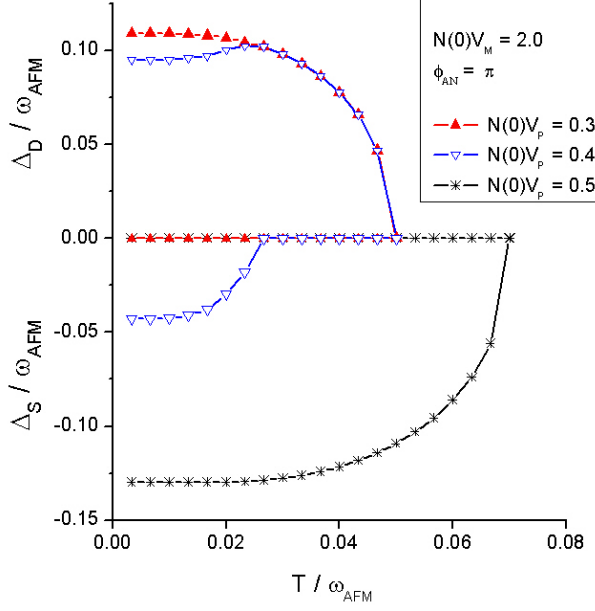


FIG. 4: (Color online) (D+iS) case. Calculated magnitudes of d-wave component (Δ_d/ω_{AFM}) and s-wave component (Δ_s/ω_{AFM}) for different strength of phonon interaction $N(0)V_p = 0.3, 0.4$, and 0.5 . For all cases $N(0)V_M = 2.0$, $\phi_{AN} = \pi$, $\omega_{ph}/\omega_{AFM} = 0.5$.

The summary for the (D+iS) type gap is: (1) The mixed type gap solution is possible if the phonon interaction $\lambda_{ph,S}$ is comparable but still subdominant to the AFM interaction strength $\lambda_{AFM,D}$. (2) In contrast to the (D+S) case, separate two transition temperatures $T_{c,D}$ and $T_{c,S}$ exist for each gap Δ_D and Δ_S ; $T_{c,D}$ is always higher than $T_{c,S}$ and only below $T_{c,S}$ two gaps coexist. (3) As in the (D+S) case, T_c is not enhanced as far as the d-wave gap remains finite regardless of the presence and magnitude of the s-wave gap component. (4) Anisotropy of the phonon interaction is not particularly necessary.

C. ($D_{AFM}+D_{ph}$) case

This is the case that phonon interaction also supports the d-wave pairing. Because it is clear that a perfectly isotropic phonon interaction has null effect on the d-wave gap, anisotropy of the phonon interaction is crucial for this case. The total gap is, therefore, $\Delta_t(\phi) = (\Delta_{d1} + \Delta_{d2}) \cos(2\phi)$ and the gap equations are written as

$$\Delta_{d1}(\phi) = - \sum_{\phi'} V_{AFM}(\phi - \phi') \Delta_t(\phi') \chi(\phi', \omega_{AFM}), \quad (13)$$

$$\Delta_{d2}(\phi) = - \sum_{\phi'} V_{ph}(\phi - \phi') \Delta_t(\phi') \chi(\phi', \omega_{ph}). \quad (14)$$

The above two gap equations can be combined to a single

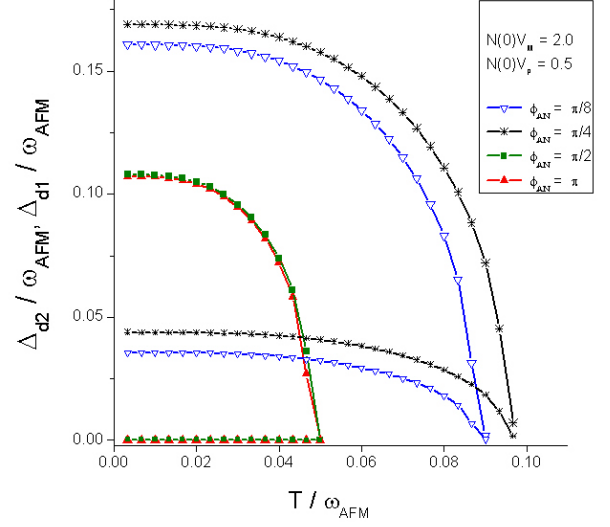


FIG. 5: (Color online) ($D_{AFM}+D_{ph}$) case. Calculated magnitudes of D_{AFM} component (Δ_{d1}/ω_{AFM}) and D_{ph} component (Δ_{d2}/ω_{AFM}) for different anisotropy angles $\phi_{AN} = \pi/8, \pi/4, \pi/2$, and π . For all cases $N(0)V_M = 2.0$, $N(0)V_p = 0.5$ and $\omega_{ph}/\omega_{AFM} = 0.5$.

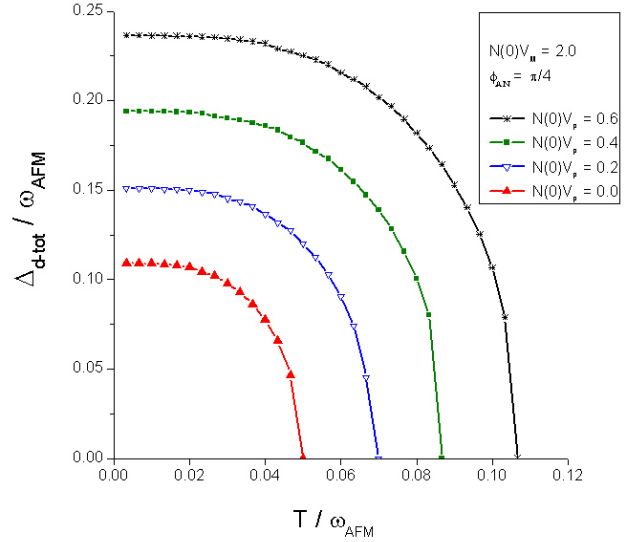


FIG. 6: (Color online) ($D_{AFM}+D_{ph}$) case. Calculated magnitudes of the total d-wave gap ($\Delta_{d-tot}/\omega_{AFM}$) for different strength of phonon interaction $N(0)V_p = 0.0, 0.2, 0.4$, and 0.6 . For all cases $N(0)V_M = 2.0$, $\phi_{AN} = \pi/4$ and $\omega_{ph}/\omega_{AFM} = 0.5$.

gap equation but we keep the separate form in order to trace the effect of the phonon interaction. In contrast to the previous cases, T_c can be dramatically enhanced when the phonon interaction $V_{ph}(\Delta\phi)$ has a proper degree of anisotropy. Other authors¹⁰ also obtained a similar result using different approaches. In Fig.5, we plot Δ_{d1} and Δ_{d2} separately; between the same symbols the smaller value is the phonon induced d-wave gap Δ_{d2} and the larger one is the AFM induced d-wave gap Δ_{d1} . We change the anisotropy angle of $V_{ph}(\Delta\phi)$ with the fixed interaction strengths of $N(0)V_M = 2.0$ ($\lambda_{AFM,D} = 0.332$) and $N(0)V_P = 0.5$. For the anisotropy angle $\phi_{AN} = \pi/2$ and π , the phonon interaction has absolutely no effect on the d-wave pairing; this is simply because the d-wave projected average Eq.(10) becomes zero for these two commensurate angles with our model potential Eq.(3). With a stronger anisotropy ($\phi_{AN} = \pi/4$; $\lambda_{ph,D} = 0.12$), the phonon scattering sees only a limited part of the d-wave gap, therefore the d-wave gap can be seen effectively as a s-wave gap for the anisotropic phonon. For a even stronger anisotropy ($\phi_{AN} = \pi/8$; $\lambda_{ph,D} = 0.098$), too narrow scattering angle reduces the effective coupling strength. In our model potential, $\phi_{AN} = \pi/4$ is the optimal anisotropy. In fact, even weaker anisotropy of $\pi/4 < \phi_{AN} < \pi$ – except the special commensurate angles $\phi_{AN} = \pi/2$ and π – produces some uncompensated effective interaction $\lambda_{ph,D}$ and boosts the d-wave pairing. This is an artifact of the model potential Eq.(10) which always emphasizes the small angle scattering. Therefore, for some real phonons, it is possible to have a repulsive (destructive for d-wave pairing) $\lambda_{ph,D}$ if large angle (around $\Delta\phi = \pi/2$) scattering overweighs small angle scattering.

Fig.6 shows the results of total gap $\Delta_{d-tot} = \Delta_{d1} + \Delta_{d2}$ with the optimal anisotropy angle $\phi_{AN} = \pi/4$ and varying phonon coupling strength $N(0)V_P = 0.0, 0.2, 0.4$, and 0.6 ($\lambda_{ph,D} = 0.0, 0.047, 0.095$, and 0.142 , respectively). The results demonstrate that the relatively weak phonon interaction $\lambda_{ph,D}$ can significantly increase T_c from the pure AFM interaction induced T_{c0} .

Considering the experimental findings about phonons in the high- T_c cuprates, the best candidate for the anisotropic pairing phonon is B_{1g} buckling mode of the plane oxygen motion². Devereaux and coworkers extensively analyzed the behaviors of B_{1g} mode and found : (1) B_{1g} mode has a strong anisotropic coupling matrix element concentrating around antinodal points; (2) the maximum coupling strength can reach as high as $\lambda \sim 3$. Compared to our model calculations, the optimal anisotropy for the d-wave pairing $\phi_{AN} = \pi/4$ is just about the same degree of anisotropy of the B_{1g} mode. Regarding the coupling strength, for example, in Fig.6 the maximum coupling strength λ_{max} is $N(0)V_P = 0.6$ and the corresponding average strength is $\lambda_{ph,D} = 0.142$. These values are much smaller than the ones extracted by Devereaux and coworkers². Larger values of coupling constants would be more realistic. However since our study is limited within the BCS gap equations we chose smaller values of coupling constants. With larger coupling strength ($\lambda > O(1)$), we should go for the strong coupling theory for the reliable analysis. Also for the same phonon, the coupling strength extracted from ARPES experiments and the coupling strength

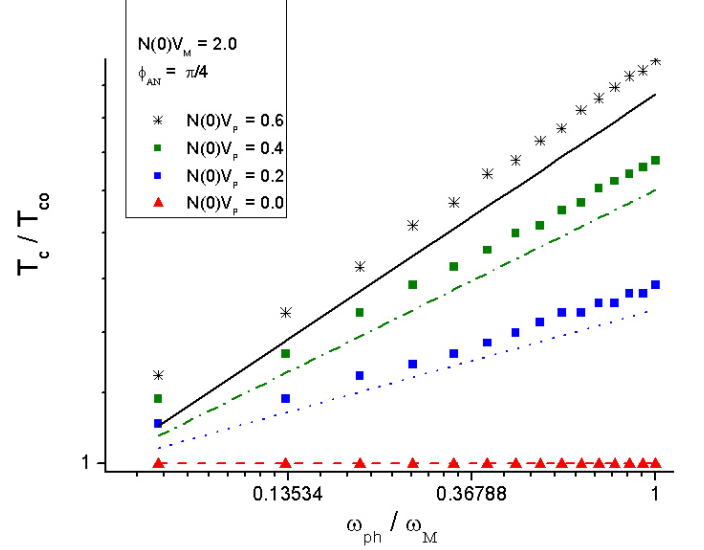


FIG. 7: (Color online) $(D_{AFM}+D_{ph})$ gap. T_c (symbols) calculated as a function of ω_{ph}/ω_{AFM} for different strength of phonon interaction $N(0)V_P = 0.0, 0.2, 0.4$, and 0.6 , normalized by T_{c0} the transition temperature with $N(0)V_P = 0.0$. For all cases, $N(0)V_M = 2.0$ and $\phi_{AN} = \pi/4$. Lines are the results of the analytic formula of T_c Eq.(15). The symbols and lines of the same colors have the same parameters set.

for the pairing problem can be very different due to the on-site Coulomb interaction.

Another important anisotropic phonon in Bi-2212 is the breathing mode which strongly interacts near the nodes. The effect of this phonon is partially included in our calculations because our model phonon interaction Eq.(3) only constraints the scattering angle by ϕ_{AN} but doesn't constraint the incoming \mathbf{k} and outgoing momenta \mathbf{k}' (ϕ and ϕ' in our model). The anisotropic phonon scattering concentrating near nodes will be mostly averaged out by the sign changing d-wave gap and will be of no importance for the d-wave pairing. For realistic estimate of the phonon effects in HTC compounds, all important phonons should be included to calculate $\lambda_{ph,D}$ using full coupling matrix elements. This is beyond the scope of the current paper.

Since we found that an anisotropic phonon can dramatically enhance T_c of d-wave pairing, we have to consider the isotope effect of the phonon, which is reported to be anomalously small, in particular, near optimal doping region by many experiments¹². For this purpose, Fig.7 shows the calculated T_c 's (symbols) from Eq.(13-14) as a function of the phonon energy cutoff ω_{ph}/ω_{AFM} for various phonon coupling strength $N(0)V_P = 0.0, 0.2, 0.4$ and 0.6 , respectively. The BCS theory predicts $T_c \sim \omega_{ph}$ ($\alpha = 0.5$), which should show up as a linear lines in Fig.7. Our numerical results show much weaker power than the linear one

indicating $\alpha < 0.5$. For more analytic investigation for the isotope effect and the origin of the T_c enhancement by phonon in the $(D_{AFM}+D_{ph})$ case, we derived an analytic T_c equation. The gap equations Eq.(13-14) can reduce to a single T_c equation by adding two equations and taking a limit of $\Delta_{d1}, \Delta_{d2} \rightarrow 0$. The pair susceptibility $\chi(\omega_{AFM,ph})$ (Eq.(9)) is integrated out using BCS approximation which is $\int_0^{\omega_D} d\xi [\tanh \frac{\xi}{2T}]/\xi \approx \ln[2C\omega_D/\pi T]$ ($C = e^\gamma \approx 1.7807$), valid when $\omega_D/2T_c \gg O(1)$. Finally we obtained the T_c formula of the $(D_{AFM}+D_{ph})$ case as

$$T_c \simeq 1.13 \omega_{AFM}^{\tilde{\lambda}_{AFM}} \cdot \omega_{ph}^{\tilde{\lambda}_{ph}} e^{-1/\lambda_t}. \quad (15)$$

where $\lambda_t = (\lambda_{AFM} + \lambda_{ph})$, $\tilde{\lambda}_{AFM} = \lambda_{AFM}/\lambda_t$ and $\tilde{\lambda}_{ph} = \lambda_{ph}/\lambda_t$, and λ_{AFM} and λ_{ph} are the dimensionless effective coupling constants obtained from Eq.(10) with d-wave gap average for both couplings. ω_{AFM} and ω_{ph} are the energy cutoffs of the AFM interaction and phonon interaction, respectively. As mentioned above, this T_c formula is derived assuming $\omega_{M,ph}/2T_c \gg O(1)$ and this condition is well satisfied when $\lambda_t < O(1)$. In Fig.7, we also plot the results of T_c 's from Eq.(15) (lines) with the same parameters and compare them with the numerical calculations (symbols) from Eq.(13-14). It shows a reasonably good agreement between two results although the deviations increase with increasing the coupling constant $N(0)V_p$ (or $\lambda_{ph,D}$) as expected. However, the overall and quantitative behavior of T_c is well captured by Eq.(15).

Now we are in position to read the phonon isotope coefficient α from Eq.(15), which is

$$\alpha = \frac{1}{2} \tilde{\lambda}_{ph} = \frac{1}{2} \frac{\lambda_{ph}}{\lambda_{AFM} + \lambda_{ph}}. \quad (16)$$

For example, with representative values of $\lambda_{AFM} = 0.33$, $\lambda_{ph} = 0.1$ and $\omega_{ph}/\omega_{AFM} = 0.5$, we obtain $\alpha \approx 0.116$, which is pretty small value compared to the standard BCS value of 0.5 while T_c is enhanced by about 100% from T_{c0} the transition temperature without phonon interaction (see Fig.7; $N(0)V_P = 0.6$ is $\lambda_{ph} = 0.142$). This isotope coefficient equation Eq.(16) provides a very plausible resolution why the isotope coefficient is so low near optimal doping region where T_c is the highest and increases toward underdoped regime (decreasing T_c). The phonon coupling strength (λ_{ph}) is likely unchanged with doping but the effective coupling strength of the AFM mediated interaction (λ_{AFM}) will change sensitively with doping. If we assume that λ_{AFM} increases with increasing doping but λ_{ph} remains constant, Eq.(16) describes the general trend of the experimentally observed oxygen isotope effect α_O^{12} .

D. $(D_{AFM}+D_{ph}+iS_{ph})$ case

Combining the $(D_{AFM}+D_{ph})$ and $(D+iS)$ case, we can consider the $(D_{AFM}+D_{ph}+iS_{ph})$ type solution. This is indeed a natural solution of the combined gap equations (12),

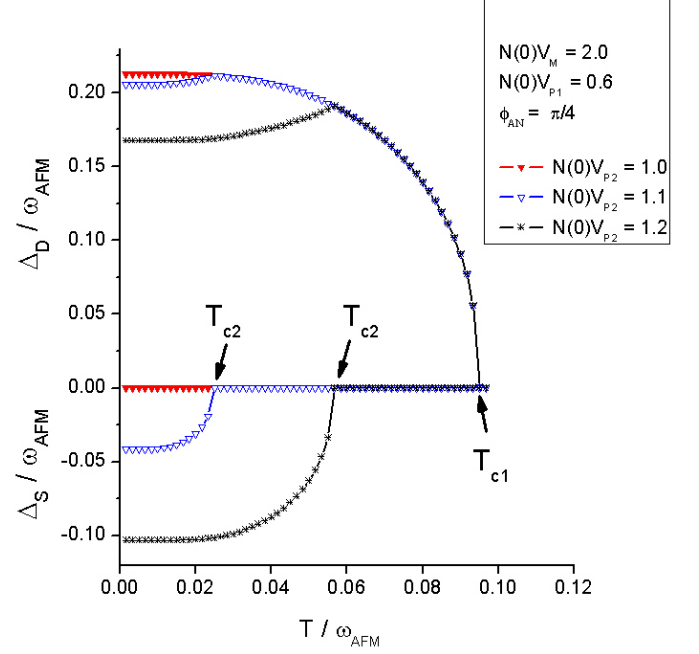


FIG. 8: (Color online) $(D_{AFM}+D_{ph}+iS_{ph})$ case. Calculated magnitudes of total d-wave component ($\Delta_D = \Delta_{AFM} + \Delta_{ph}$) and s-wave component (Δ_s) for different strength of phonon interaction $N(0)V_{P2} = 1.0, 1.1$ and 1.2 . For all cases $N(0)V_M = 2.0$, $N(0)V_{P1} = 0.6$, $\phi_{AN} = \pi/4$, and $\omega_p/\omega_{AFM}=0.5$.

(13), and (14) and the total gap will be $\Delta_t(\phi) = (\Delta_{d1} + \Delta_{d2}) \cos(2\phi) + i\Delta_s$. In this case, phonon interaction(s) mediate both d-wave and s-wave pairings, which seems contradicting to a common knowledge. The fact is that phonon alone - no matter how anisotropic - cannot induce a d-wave gap but it can boost it if a d-wave gap is formed by other interaction. Then as we found in the $(D+iS)$ section, a phonon interaction can add iS component at lower temperatures. The interesting point is that the phonon interaction boosting d-wave gap and the phonon interaction inducing iS gap can originate from the same phonon if the anisotropy and the interaction strength are properly tuned. Of course more general case is that two different phonon modes play separate roles, respectively. For clearness, we rewrite the gap equations describing $(D_{AFM}+D_{ph}+iS_{ph})$ case below.

$$\Delta_{d1}(\phi) = - \sum_{\phi'} V_{AFM}(\phi - \phi') \Delta_t(\phi') \chi(\phi', \omega_{AFM}) \quad (17)$$

$$\Delta_{d2}(\phi) = - \sum_{\phi'} V_{1,ph}(\phi - \phi') \Delta_t(\phi') \chi(\phi', \omega_{p1}), \quad (18)$$

$$i\Delta_s(\phi) = - \sum_{\phi'} V_{2,ph}(\phi - \phi') \Delta_t(\phi') \chi(\phi', \omega_{p2}) \quad (19)$$

where the pair susceptibilities $\chi(\phi, \omega)$ are defined in Eq.(9) and the quasiparticle energy is $E(\phi) = \sqrt{\xi^2 + \Delta_d^2(\phi) + \Delta_s^2}$ with $\Delta_d(\phi) = (\Delta_{d1} + \Delta_{d2}) \cos(2\phi)$. For generality we

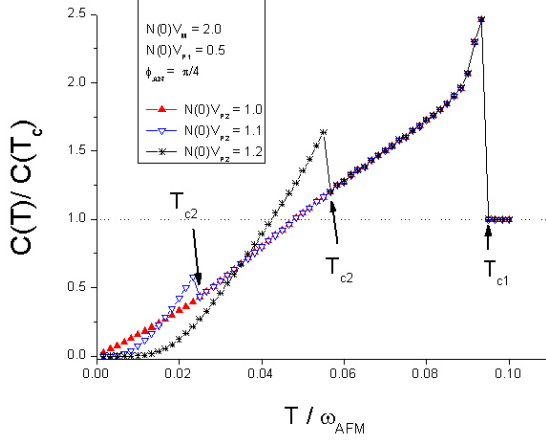


FIG. 9: (Color online) ($D_{AFM} + D_{ph} + i S_{ph}$) case. Normalized specific heats $C(T)/C(T_c)$ for different strength of phonon interaction $N(0)V_{P2}$. There are two transition temperatures T_{c1} (higher) and T_{c2} (lower). Same parameters as in Fig.8.

assume two different phonon interactions $V_{1,ph}$ and $V_{2,ph}$, respectively but they can be the same phonon as explained above.

In Fig.8 we plot the solutions of $\Delta_d = \Delta_{d1} + \Delta_{d2}$ and Δ_s components separately. We fix the AFM interaction $N(0)V_M=2.0$ and the d-wave boosting phonon interaction $N(0)V_{P1}=0.6$ as a case of Fig.6 and vary the phonon interaction $N(0)V_{P2}$ inducing iS gap component as 1.0, 1.1, and 1.2, respectively. T_c is enhanced by $N(0)V_{P1}$ and doesn't change for different $N(0)V_{P2}$ values because it is determined only by the d-wave gap component. We also chose the same anisotropy $\phi_{AN} = \pi/4$ for both phonons $V_{1,ph}$ and $V_{2,ph}$ for convenience. Anisotropy condition for the d-wave boosting phonon is important; optimal anisotropy is $\phi_{AN} = \pi/4$ for our model. However, the phonon interaction $V_{2,ph}$ inducing iS gap doesn't need to be anisotropic.

This type of gap solution can provide a possible resolution to the recent experiments of HTC which indicate the presence of a s-wave component at low temperatures. The anomalous tunnelling conductance in YBCO³, non-monotonic behavior of the penetration depth at low temperatures and its isotope effect⁴, etc indicate a mixed gap of the (D+ iS) type at low temperatures and a phonon effect with it. Fig.9 show the normalized specific heat $C(T)/C(T_{c1})$ for the gap solutions of Fig.8. General feature is that it shows a d-wave type specific heat below T_{c1} and then turns into a s-wave type behavior below T_{c2} where iS gap component opens. Since the second transition at T_{c2} is a true second order phase transition, the specific heat exhibits a jump. But the size of jump is far smaller than the BCS value of $\Delta C = 1.43 C(T_{c2})$. The reason is because when iS gap opens at T_{c2} , the magnitude of d-wave gap also abruptly decreases so that the amount of the specific heat jump is partially cancelled. Nevertheless, careful experiments should be able to discern the jump in the specific

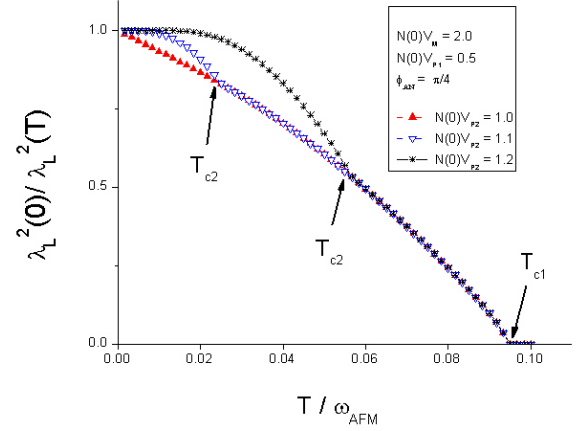


FIG. 10: (Color online) ($D_{AFM} + D_{ph} + i S_{ph}$) case. Normalized superfluid density $\lambda_L^2(0)/\lambda_L^2(T)$ for different strength of phonon interaction $N(0)V_{P2}$. Same parameters as in Fig.8.

heat at the second transition temperature T_{c2} if this scenario is true.

Fig.10 shows the normalized superfluid density $\lambda_L^2(0)/\lambda_L^2(T)$ for the gap solutions of Fig.8. The general features are the same as in the specific heat: d-wave behavior in between T_{c1} and T_{c2} , and s-wave behavior below T_{c2} . In particular, the additional sharp increase of $\lambda_L^{-2}(T)$ below T_{c2} has some resemblance to the experimental observations⁴ although the flattened out behavior at very low temperatures is not clearly observed experimentally.

We propose a firm experimental test for this scenario. The d-wave boosting phonon interaction does not have a minimum interaction strength; as far as it has a proper anisotropy it will enhance the d-wave pairing as much as with its strength. For the iS component to appear below T_{c2} the phonon interaction needs a minimum strength to overcome a part of d-wave component. Therefore, a controlled suppression of d-wave gap (with non-magnetic impurities not to weaken the s-wave pairing) will widen a window of low temperature region where the iS component pops up.

III. CONCLUSIONS

In this paper we studied the effects of phonon interaction on the superconducting pairing in the background of d-wave gap already formed by the AFM interaction. In particular, we studied the role of anisotropy of the phonon interaction and possible multigap type solutions within a generalized BCS theory. For many cases the anisotropy of the phonon interaction is a crucial condition for interesting interplay with the AFM interaction but not always; the (D+S) type gap need anisotropic phonon but (D+ iS) type gap is more tolerable with the anisotropy of phonon interaction because two gaps are more gently coupled in the (D+ iS) case. In both cases, T_c is

not enhanced at all by phonon interaction as far as the d-wave gap component remains finite.

Anisotropic phonon can boost T_c together with the AFM interaction in the $(D_{AFM} + D_{ph})$ type solution. With numerical calculations and analytic T_c equation, we showed that T_c is enhanced dramatically following the modified BCS exponential form $T_c \sim \exp(-1/\lambda_t)$ with the total coupling strength $\lambda_t = \lambda_{AFM} + \lambda_{ph}$. This type of solution can also explain how and why the phonon isotope effect is strongly reduced despite the large enhancement of T_c by phonon. Our isotope coefficient formula Eq.(16) provides a good description of the overall trend of oxygen isotope coefficient α_O ¹².

Also a combined type solution of $(D_{AFM} + D_{ph} + iS)$ gap is considered. This type of gap not only shows the features of the $(D_{AFM} + D_{ph})$ gap – enhanced T_c and small isotope effect – but also shows the appearance of a s-wave component at low temperatures. The latter feature can provide a microscopic origin of the small s-wave component suggested from recent experiments of tunnelling conductance³ and penetration depth measurements⁴. Calculations of the superfluidity density showed a qualitative agreement with experiments of the abrupt increase of $\lambda_L^{-2}(T)$ at lower temperatures⁴. However, this scenario should be confirmed by experimental observation of a specific heat jump at the second low transition

temperature T_{c2} for the s-wave gap component as shown in Fig.9. We proposed a systematic impurity doping study to test this scenario.

Finally, we would like to restate the limitation of our work. First, the dynamical interplay between phonon(s) and AFM interaction is not properly treated. This problem was already studied by many authors^{9,10,11}. We bypassed this complicated problem on the phenomenological basis; after all correlation effects taken place we assumed that fermion quasiparticles remain, and AFM spin fluctuations and several phonon modes are considered as experimentally defined quantities after mutual screening and renormalization. Second, when we consider the s-wave pairing, we should have included the on-site Coulomb interaction in the HTC cuprates in addition to the phonon interaction. Therefore, $\lambda_{ph,S}$ in this paper should be considered as a renormalized quantity after including the on-site Coulomb interaction. Perhaps, this is the reason why our $\lambda_{ph,S}$ (~ 0.1) is order of magnitude smaller than the experimental values² $\lambda_{exp} \sim O(1)$.

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